Finite Extension of Polymers in Turbulent Flow

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The statistics of polymers advected by a turbulent flow are investigated. To limit the polymer lengths above to coil–stretch transition, a FENE-P type relaxation law is used. The turbulence is modeled by a random strain, delta-correlated in time and with Gaussian statistics. The distribution of polymer lengths for both the coiled and stretched states are derived, from which are obtained analytical expressions for the moments of the distribution. The polymer stress on the fluid decreases linearly with the inverse of the Deborah number. The degradation (breaking) of the polymers is also discussed, showing that even for large Deborah number some polymers can remain unbroken.

One of the principal motivations to study the properties of polymers diluted in a turbulent flow is to understand the Toms effect, also known as drag reduction [1, 2], whereby the effect of a small concentration of polymers is to dramatically reduce the pressure required to maintain a turbulent flow at a given velocity in a pipe. It is thought that the extension of the polymers by the strains in the turbulent flow (the coil–stretch transition) is crucial to that effect [1, 3]. More recently, there has been great progress in understanding the microscopic behavior of biological polymers such as DNA [4–6], which give confidence that there is a regime where the polymer tension dominates the relaxation time [7], as opposed to hydrodynamic effects.

The dynamics of polymers in incompressible turbulence was studied recently in Refs. [8–11]. Balkovsky et al. [8, 10], building on the approach of Lumley [12], modeled the turbulence as a homogeneous, isotropic, delta-correlated random strain—the Kraichnan–Kazantsev model of turbulence [13–18] (see the review by Falkovich et al. [19])—for polymers whose relaxation is described by the Hookean dumbbell model [20]. Chertkov [9] extended the analysis to general nonlinear relaxation models. Experiments [11] and numerical simulations [21] validate many of the findings of these papers.

In this letter we explore the coiled and stretched states of polymers assuming the popular FENE-P model [20, 22, 23] (Finite Extension Nonlinear Elastic) for the relaxation force of the polymer. The advantage of the FENE model is that its nonlinear nature prevents the polymers from being infinite in length above the coil–stretch transition: it limits them to a finite, fixed length. The results for the PDF of the polymer lengths in both the coiled and stretched states are presented, as well as moments of the distribution, the polymer stress on the fluid, and a discussion of polymer degradation by breaking. For

definiteness and simplicity, Gaussian statistics for the strain are assumed throughout, though the calculation herein could be redone for more arbitrary statistics using the path integral formalism used by Chertkov [9]. The emphasis is thus on presenting closed form, analytically simple expressions that give a reasonable description of the physics. Compressibility effects are neglected, as is the feedback of the polymers on the flow, justified when the polymer stress is much less than $\nu\bar{\lambda}$ [8], where ν is the fluid (Newtonian) viscosity and $\bar{\lambda}$ is the mean rate of strain.

I. FOKKER–PLANCK EQUATION

The shape of the polymers is characterized by the symmetric conformation tensor, $\mathbb{A}$, which describes the deformation of the polymers from a coiled ball of radius ρ_0 into a stretched ellipsoid in the presence of flow. We take the equation of motion for the conformation tensor to be that of a general viscoelastic fluid with a relaxation force term (only the longest restoring time is taken into account),

$$\frac{dA^{ij}}{dt} = A^{ik}\,\partial_k u^j + \partial_k u^i A^{kj} - \frac{2}{\tau}\left(f(A^{kk})A^{ij} - \rho_0^2\,\delta^{ij}\right),$$
(1)

where $f(A^{kk})$ depends only on the trace A^{kk} of $\mathbb{A}$, and is equal to 1 when $\mathbb{A} = \rho_0^2\,\mathbb{I}$, and $d/dt = \partial/\partial t + u^k\partial_k$ is the advective derivative. We take the velocity field to be incompressible, $\partial_k u^k = 0$. (Unless otherwise noted, repeated indices are summed.) The conformation tensor $\mathbb{A}$ can be diagonalized, with eigenvalues ρ_α^2 that evolve according to

$$\frac{d\rho_\alpha}{dt} = \hat{\sigma}_{\alpha\alpha}\,\rho_\alpha - \frac{1}{\tau}\left(f(\rho_\beta\rho_\beta)\rho_\alpha - \rho_0^2/\rho_\alpha\right),$$
(2)

with $\hat{\sigma}_{\alpha\beta}(t,\boldsymbol{x}) := \boldsymbol{e}_\alpha^i\,\partial_k u^i\,\boldsymbol{e}_\beta^k$ the velocity gradient tensor projected on the orthonormal eigenvectors, $\boldsymbol{e}_\alpha$. There is no sum over α on the right-hand side of (2).

When the viscous scale of the flow is much larger than the polymer length (the typical situation), the turbulence appears locally as a constant strain. In the context of our

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model, the polymers are stretched ellipsoids whose major axis is aligned with the dominant stretching direction, associated with the largest Lyapunov exponent, positive here for an incompressible flow. This alignment is observed in numerical experiments [23]. We thus neglect the subdominant directions in (2) and write

$$\frac{d\rho}{dt} = \lambda\rho - \frac{1}{\tau}\left(f(\rho^2)\rho - \rho_0^2/\rho\right),\qquad(3)$$

where ρ is the largest ρ_α and $\lambda(t)$ is the Lyapunov exponent associated with the dominant direction of stretching.

We take $\lambda(t)$ to be a random variable satisfying

$$\langle\lambda(t)\lambda(t')\rangle - \bar\lambda^2 = \delta(t-t')\,\Delta;\qquad \langle\lambda(t)\rangle = \bar\lambda,\qquad(4)$$

where the angle brackets denote a average over $\lambda(t)$. In general we have $\Delta \le \bar\lambda$, since the standard deviation cannot be larger than the mean for the positive Gaussian variable λ.

To get a Fokker–Planck equation for the PDF of ρ, we introduce the characteristic function, $\mathcal{Z}(t;\mu) = \langle\exp(\mathrm{i}\mu\rho)\rangle$. We can then derive an equation of motion for $\mathcal{Z}$ from (3) and average. Gaussian integration by parts [24–27] allows evaluation of terms of the form $\langle\lambda\mathcal{Z}\rangle$, finally yielding a closed equation for $\mathcal{Z}$. Inverse Fourier transformation of $\mathcal{Z}$ with respect to μ then gives the equation of motion for $\mathcal{P}(t,\rho)$, the PDF of ρ,

$$\partial_t\mathcal{P} = \tfrac{1}{2}\Delta\,\partial_\rho\rho\,\partial_\rho\rho\,\mathcal{P} - \bar\lambda\,\partial_\rho\,\rho\,\mathcal{P} + \frac{1}{\tau}\,\partial_\rho\left(f(\rho^2)\rho - \rho_0^2/\rho\right)\mathcal{P}.\qquad(5)$$

(The ∂_ρ act on all terms to their right.) This is the same Fokker–Planck equation as derived by Chertkov [9], except that instead of diffusivity we shall use the minimum polymer size ρ_0 as an ultraviolet cutoff. This also allows us to treat the coiled state in Section II.

II. THE COILED STATE

We first deal with the case of relatively unstretched polymers, so that their effective radius (the maximal extension of the ellipsoid describing the deformation of the polymers) is much less than the maximal extension of the polymer. In that case we assume that the polymers are in a linear force response regime and we can use the Hookean dumbbell model, $f(\rho^2) = 1$. Since the determinant of $\mathbb{A}$ is greater than $(\rho_0^3)^2$ (see the appendix), we can assume that the largest principal axis ρ (the only one we model) is larger that ρ_0, and assume the PDF of ρ vanishes for $\rho < \rho_0$.

The Fokker–Planck equation (5) with $f = 1$ can be solved for the steady-state distribution,

$$\mathcal{P}_c(\rho) \sim \rho^{-1-2(\xi-\zeta)}\exp(-\xi\,\rho_0^2/\rho^2),\qquad(6)$$

where $\xi := 1/\Delta\tau$, $\zeta := \bar\lambda/\Delta$. From the PDF we can derive an exact expression for its moments,

$$\frac{\langle\rho^n\rangle}{\rho_0^n} = \xi^{n/2}\,\frac{\gamma(\xi-\zeta-n/2,\xi)}{\gamma(\xi-\zeta,\xi)},\qquad(7)$$
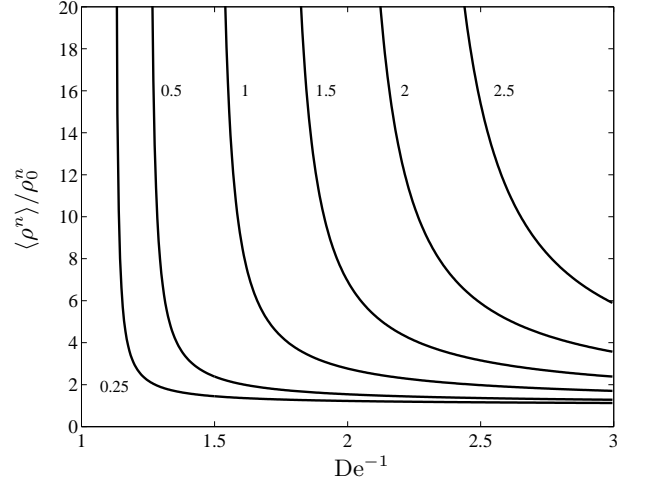

FIG. 1: Moments $\langle\rho^n\rangle/\rho_0^n$ of the PDF of polymer lengths in the coiled state for different values of n, with $\zeta := \bar\lambda/\Delta = 1$.

where $\gamma(a,x)$ is the lower incomplete gamma function. ($\gamma(a,\infty)$ is equal to $\Gamma(a)$, the complete gamma function.) For $\xi > \zeta$, the denominator in (7) is positive and finite, and for $n < 2(\xi-\zeta)$ so is the numerator.

For $n = 2(\xi-\zeta)$ the numerator diverges, so that the moment $\langle\rho^n\rangle$ becomes infinite. When $\xi = \zeta$ the $n = 0$ moment diverges, which means that the PDF $\mathcal{P}_c$ becomes unnormalizable. Thus the physical picture is as follows: for large $\xi - \zeta$ only moments associated with large n diverge, but as $\xi - \zeta$ is lowered more moments diverge, indicating that on average more polymers have anomalously long lengths, that is, they are uncoiled. For $\xi = \zeta$ all positive ($n > 0$) moments are infinite, which indicates that the polymers are essentially all in a stretched (uncoiled) state, but also pointing to a breakdown in the theory because of the infinite moments.

The combination $\xi - \zeta$ can be rewritten

$$\xi - \zeta = \zeta(\mathrm{De}^{-1} - 1);\qquad \mathrm{De} := \bar\lambda\tau,\qquad(8)$$

where De is the Deborah number, the ratio of the polymer relaxation timescale over the advection timescale. The transition to the stretched state thus occurs for $\mathrm{De} \ge 1$. A few moments are plotted as a function of the Deborah number in Fig. 1, showing their divergence as De approaches unity.

For $\zeta + 1$ moderately large (fluctuations are small compared to the mean), the main contribution to the integral representation of the incomplete gamma function occurs well below ξ, so we can replace the upper integration bound ξ by ∞ in (7) and obtain

$$\frac{\langle\rho^n\rangle}{\rho_0^n} \simeq \xi^{n/2}\,\frac{\Gamma(\xi-\zeta-n/2)}{\Gamma(\xi-\zeta)}.\qquad(9)$$

The even moments then reduce to simple products of monomial factors according to the factorial property of

the gamma function. A simplification occurs for $n = 2$,

$$\frac{\langle \rho^2 \rangle}{\rho_0^2} \simeq \frac{\xi}{\xi - \zeta - 1} = [1 - \Delta(\bar{\lambda} + \tau)]^{-1}. \quad (10)$$

This is a particularly significant moment, since the polymer stress on the fluid is proportional to $\mathbb{A} \sim \rho^2$.

Note that the singular denominator in (10), which comes from the gamma function numerator of (9), implies that the polymer length can be much larger than ρ_0 even below the coil–stretch transition. Of course, when it becomes too large we must include nonlinear contributions to the relaxation force, the topic of the next section.

III. THE STRETCHED STATE

As we saw in Section II, the Hookean dumbbell model fails once the Deborah number reaches unity, because it cannot prevent the polymers from becoming infinitely long [3]. One standard way to prevent this is to use the FENE-P model [20, 22, 23], for which

$$f(\rho^2) = \frac{\rho_{\mathrm{m}}^2 - \rho_0^2}{\rho_{\mathrm{m}}^2 - \rho^2}. \quad (11)$$

The restoring force of the polymers is now such as to limit their length to ρ_{m} (though they make break before reaching that length, as we see below). We assume that the elongation of the polymers is smaller than the viscous length, so that their length is limited by their own elasticity and not by the hydrodynamic mechanism of Tabor and de Gennes [28, 29].

Since in this section we are interested in the stretched state of long polymers, we may neglect $\rho_0 \ll \rho_{\mathrm{m}}$ both in (5) and (11), which leads to the stationary distribution

$$\mathcal{P}_{\mathrm{s}}(\rho) \sim \rho^{-1-2(\xi-\zeta)}(1 - \rho^2/\rho_{\mathrm{m}}^2)^{\xi} \quad (12)$$

Unlike the distribution obtained in [9, 10], this PDF exhibits a cutoff at ρ_{m}, reflecting the fact the limited size of the polymers. We also impose a cutoff at ρ_0 for small ρ, because ρ cannot be less than the equilibrium length ρ_0 (see the appendix). In Ref. [9] diffusivity was used to regularize the PDF at small ρ, but both methods are equivalent since ρ_0 drops out in our approximation.

The moments of the PDF (12) are found to be

$$\frac{\langle \rho^n \rangle}{\rho_{\mathrm{m}}^n} = \frac{\Gamma(\zeta - \xi + n/2)\,\Gamma(\zeta + 1)}{\Gamma(\zeta - \xi)\,\Gamma(\zeta + 1 + n/2)} = \frac{(\zeta - \xi)_{n/2}}{(\zeta + 1)_{n/2}}, \quad (13)$$

where $(x)_n := \Gamma(x + n)/\Gamma(x)$ is the Pochhammer symbol. This expression is valid for $\zeta - \xi > 0$, or equivalently for $\mathrm{De} > 1$. At $\mathrm{De} = 1$, Eq. (13) predicts zero length for the polymers, but this is just a symptom of the neglect of ρ_0. Rather, the coiled solution of Section II must then be used.

For $n = 2$, Eq. (13) again takes a simplified form,

$$\frac{\langle \rho^2 \rangle}{\rho_{\mathrm{m}}^2} = \frac{\zeta - \xi}{\zeta + 1} = \frac{\bar{\lambda} - \tau^{-1}}{\bar{\lambda} + \Delta} = \frac{1 - \mathrm{De}^{-1}}{1 + \zeta^{-1}}, \quad (14)$$
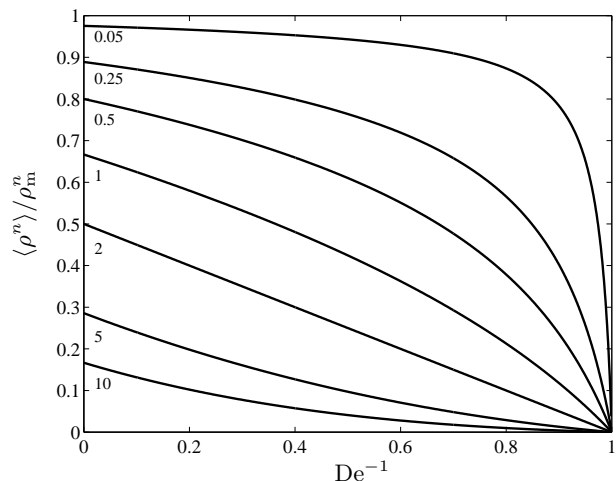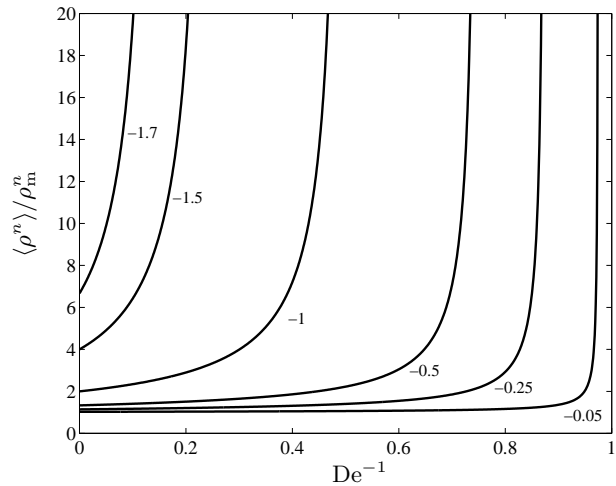

FIG. 2: Positive moments $\langle \rho^n \rangle / \rho_{\mathrm{m}}^n$ of the PDF of polymer lengths in the stretched state, with $\zeta := \bar{\lambda}/\Delta = 1$.

FIG. 3: Negative moments $\langle \rho^n \rangle / \rho_{\mathrm{m}}^n$ of the PDF of polymer lengths in the stretched state, with $\zeta := \bar{\lambda}/\Delta = 1$.

so the average polymer stress (proportional to $\langle \rho^2 \rangle$) is linear in the inverse Deborah number. Some positive ($n > 0$) and negative ($n < 0$) moments are plotted as a function of the Deborah number in Figs. 2–3. The negative moments diverge as De approaches unity, a consequence of the neglect of ρ_0.

As mentioned in Ref. [9], the PDF of length can also be used to estimate the fraction of polymers that break. (This is a kind of degradation, though not the same as say for DNA, where the two strands become separate [30].) Assume a polymer breaks if the tension $F(\rho^2) = f(\rho^2)\rho/\tau$ exceeds a critical value, F_{c}. To that critical tension corresponds a critical length, ρ_{c}, obtained by solving

$$F_{\mathrm{c}} = \frac{1}{\tau} f(\rho_{\mathrm{c}}^2)\rho_{\mathrm{c}} = \frac{1}{\tau} \frac{\rho_{\mathrm{m}}^2}{\rho_{\mathrm{m}}^2 - \rho_{\mathrm{c}}^2} \rho_{\mathrm{c}}, \quad (15)$$

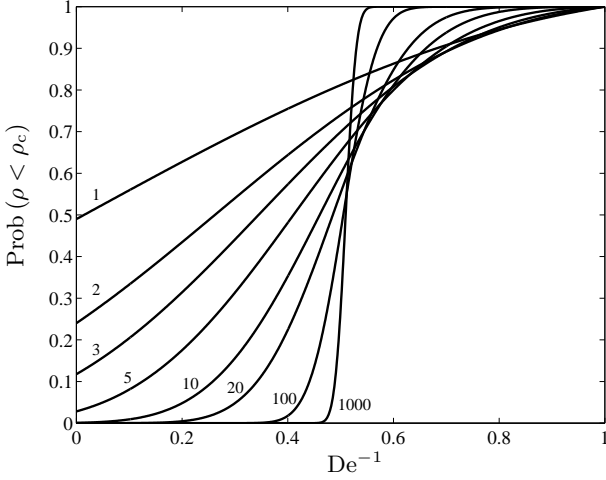a quadratic in ρ_{c}. The fraction of polymers that sur-

FIG. 4: Fraction of polymers that survive as a function of the inverse Deborah number, for different values of $\zeta := \bar{\lambda}/\Delta$ with $\rho_c/\rho_m = 0.7$.
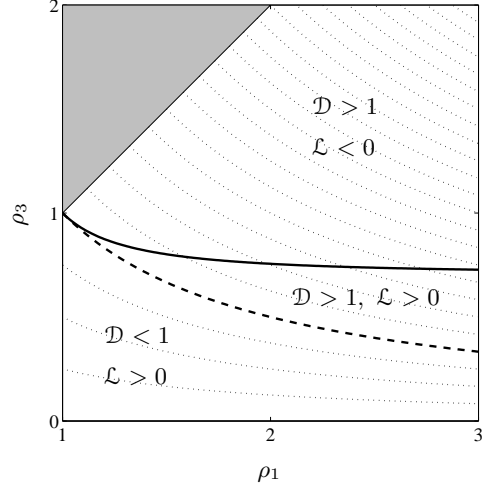

FIG. 5: Stability diagram showing that $\mathcal{D} := \rho_1\rho_2\rho_3$ must have value greater than or equal to unity. Constant-$\mathcal{D}$ curves are dotted, with the $\mathcal{D} = 1$ curve dashed.

vive is equal to the fraction shorter than ρ_c, obtained by integrating the PDF (12) from 0 to ρ_c,

$$\text{Prob}\,(\rho < \rho_c) = \frac{B(\rho_c^2/\rho_m^2\,;\,\zeta - \xi,\,\xi + 1)}{B(\zeta - \xi,\,\xi + 1)}, \qquad (16)$$

where $B(a,b) := \Gamma(a)\Gamma(b)/\Gamma(a+b)$ is the beta function, and $B(z; a, b)$ is the incomplete beta function. Since $B(1; a, b) = B(a, b)$, for $\rho_c = \rho_m$ none of the polymers break. The fraction of surviving polymers (16) is plotted in Fig. 4 for different values of ζ. For large ζ (small fluctuations), the survival probability becomes a step function with "knee" at $\text{De}^{-1} = 1 - (\rho_c/\rho_m)^2$: either all polymers survive or all are broken.

A consequence of (16) is that a significant fraction of polymers can survive even for large Deborah number; For $\xi \ll \zeta$ (De $\gg 1$) and $\xi \ll 1$, $\text{Prob}\,(\rho < \rho_c) \simeq (\rho_c/\rho_m)^{2\zeta}$, which is not small if ζ is not too large. In other words, some polymers survive breakage for large $\bar{\lambda}$ if the fluctuations in $\bar{\lambda}$ (given by Δ) are also large. Of course, this treatment is for one correlation time of the turbulence. In reality a given polymer is likely to be exposed to many different random strains. Because we have assumed the turbulence to be delta-correlated, the probability of survival of the polymers decays roughly as $(\rho_c/\rho_m)^{2\zeta N}$, where $N = t/t_{\text{corr}}$ with t the elapsed time and t_{corr} the correlation time. (More generally, for smaller Deborah number, take the Nth power of (16).)

APPENDIX: LOWER BOUND ON POLYMER VOLUME

We show that the evolution equation (1) for the polymers implies a lower limit on the volume of the polymer ellipsoid. That volume is proportional to $\det \mathbb{A} = \rho_1^2\rho_2^2\rho_2^2$,

so we let $\mathcal{D} := \rho_1\rho_2\rho_3$. (We rescale ρ such that $\|\rho_0\| = 1$.) For small volumes (low stretching) the Hookean approximation applies, so we let $f = 1$ in (2); the quantity $\log \mathcal{D}$ obeys

$$\tau \frac{d}{dt} \log \mathcal{D} = -3 + \left(\rho_1^{-2} + \rho_2^{-2} + \rho_3^{-2}\right) =: \mathcal{L}(\rho). \qquad (17)$$

The sign changes of the derivative of $\log \mathcal{D}$ are the same as those of $\mathcal{D}$ since the logarithm is monotonically increasing. Figure 5 shows the sign of $\mathcal{L}$ in the ρ_1–ρ_3 plane, assuming $\rho_2 = 1$. Without loss of generality we also assume $\rho_1 \geq \rho_3$, so we need not consider the shaded area. The solid curve is $\mathcal{L} = 0$, where the determinant is constant. The dotted curves show lines of constant $\mathcal{D}$, the dashed line being $\mathcal{D} = 1$. The dotted and dashed curves meet at the spherical solution. Below the solid curve, $\mathcal{D}$ must increase, and above it must decrease. The line $\mathcal{D} = 1$ lies entirely below $\mathcal{L} = 0$ and is tangent to it at $\rho_1 = \rho_3 = 1$. Assuming that the polymers are initially in the spherical (rest) state, we see that $\mathcal{D}$ must either remain at or increase away from unity. In fact the only disturbances that do not linearly decay back to the spherical state are those along the solid line. The picture for $\rho_2 \neq 1$ is three-dimensional but is qualitatively the same. We conclude that $\mathcal{D} \geq 1$, so that the volume of the ellipsoid is no smaller than the equilibrium sphere. Hence, the largest polymer dimension, ρ_1, is never smaller than ρ_0, justifying its use as a small-ρ_1 cutoff.

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